

PRIORITIZATION OF COMBINATORIAL LIBRARY SCREENING

ABSTRACT OF THE DISCLOSURE

In a computational method of assessing a combinatorial library for complementarity to a target molecule, ligands from the library are first docked to the target molecule. The docking results are clustered using as a metric the rms deviation between the core of two docked molecules. The library is rated as to complementarity to the target molecule according to the relative number of ligands in the top cluster.